Lecture 9: Two-Layer Neural Nets

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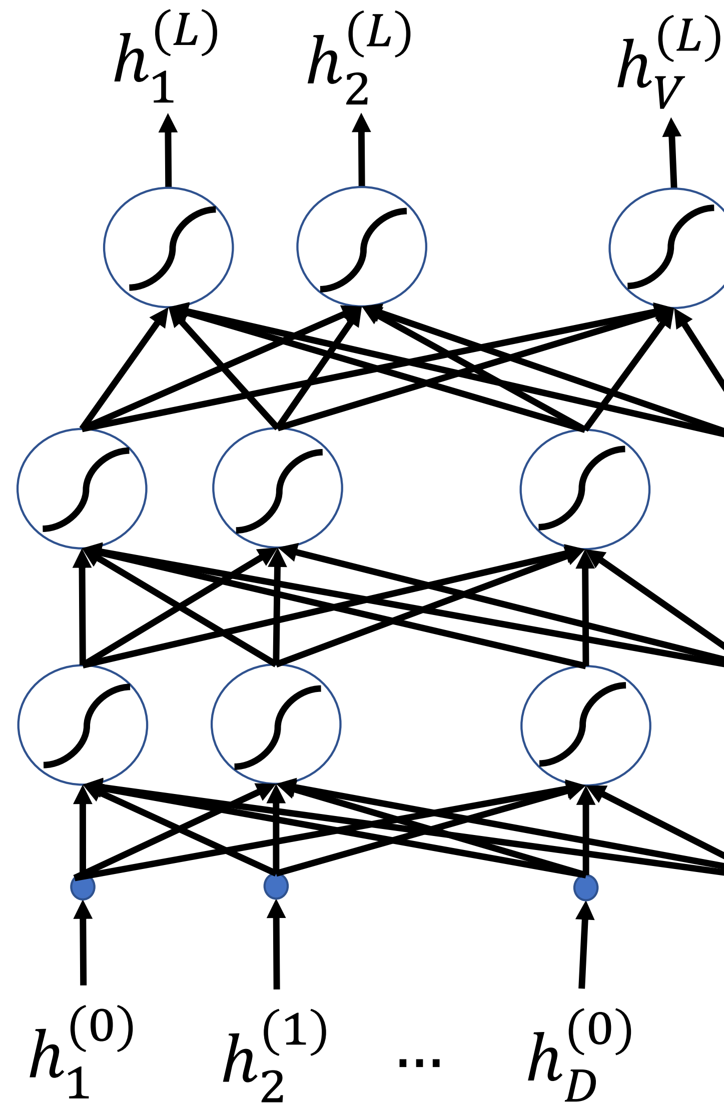
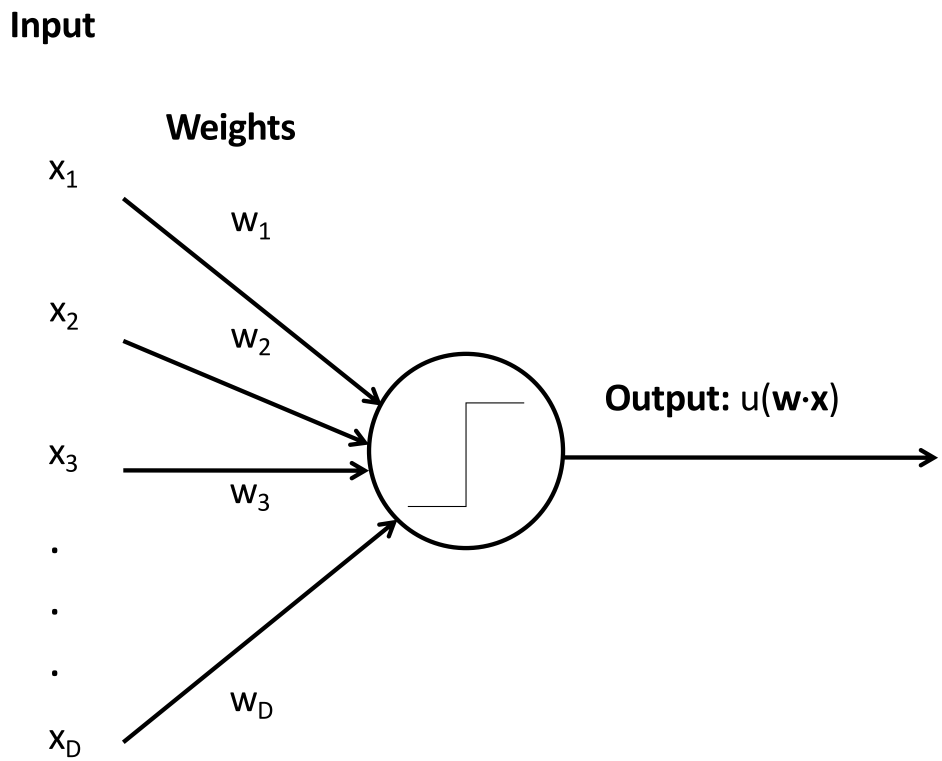


Outline

- Breaking the constraints of linearity: multi-layer neural nets
- Flow diagram for the XOR problem
- Flow diagram for a multi-layer neural net
- Forward-propagation example

Biological Inspiration: McCulloch-Pitts Artificial Neuron, 1943



- In 1943, McCulloch & Pitts proposed that biological neurons have a nonlinear activation function (a step function) whose input is a weighted linear combination of the currents generated by other neurons.
- They showed lots of examples of mathematical and logical functions that could be computed using networks of simple neurons like this.

Biological Inspiration: Neuronal Circuits

- Even the simplest actions involve more than one neuron, acting in sequence in a neuronal circuit.
- One of the simplest neuronal circuits is a reflex arc, which may contain just two neurons:
  - The **sensor neuron** detects a stimulus, and communicates an electrical signal to …
  - The **motor neuron**, which activates the muscle.

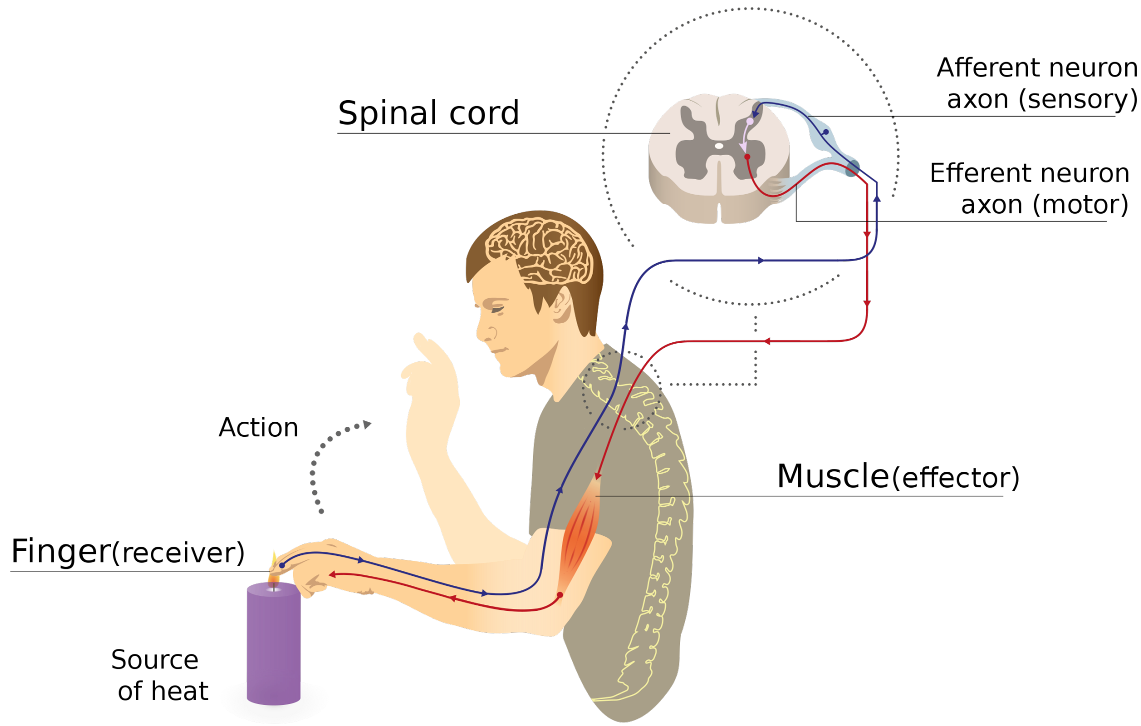


Illustration of a reflex arc: sensor neuron sends a voltage spike to the spinal column, where the resulting current causes a spike in a motor neuron, whose spike activates the muscle.

A McCulloch-Pitts Neuron can compute some logical functions…

When the features are binary ($x_j \in \{0,1\}$), many (but not all!) binary functions can be re-written as linear functions. For example, the function

$$f(\vec{x}) = (x_1 \vee x_2)$$

can be re-written as

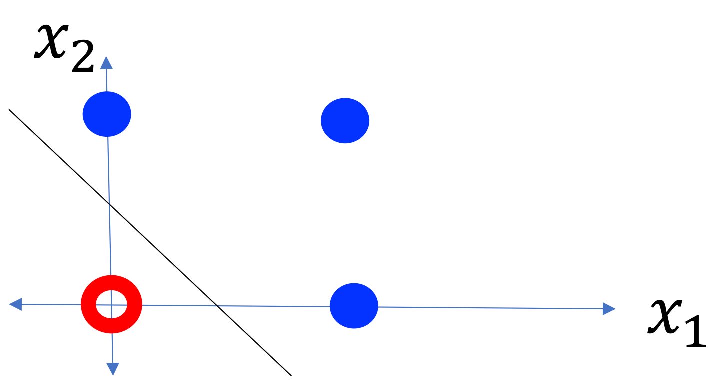
$$f(\vec{x}) = u(x_1 + x_2 - 0.5)$$

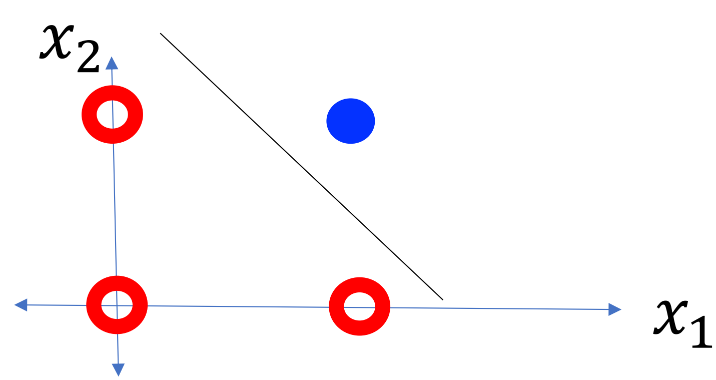
Similarly, the function

$$f(\vec{x}) = (x_1 \wedge x_2)$$

can be re-written as

$$f(\vec{x}) = u(x_1 + x_2 - 1.5)$$



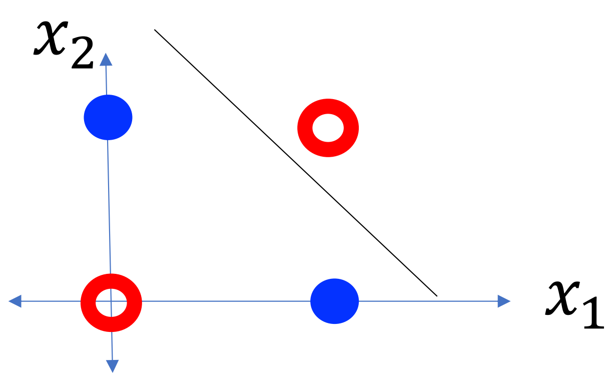


... but not all.

"A linear classifier cannot learn an XOR function."

- Minsky & Papert, 1969

- ...but a ***two-layer neural net*** can compute an XOR function!



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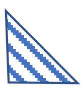
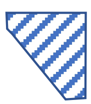
Example: one way (of many possible ways) to represent the XOR function using a two-layer neural network

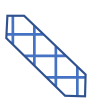
For example, consider the XOR problem.

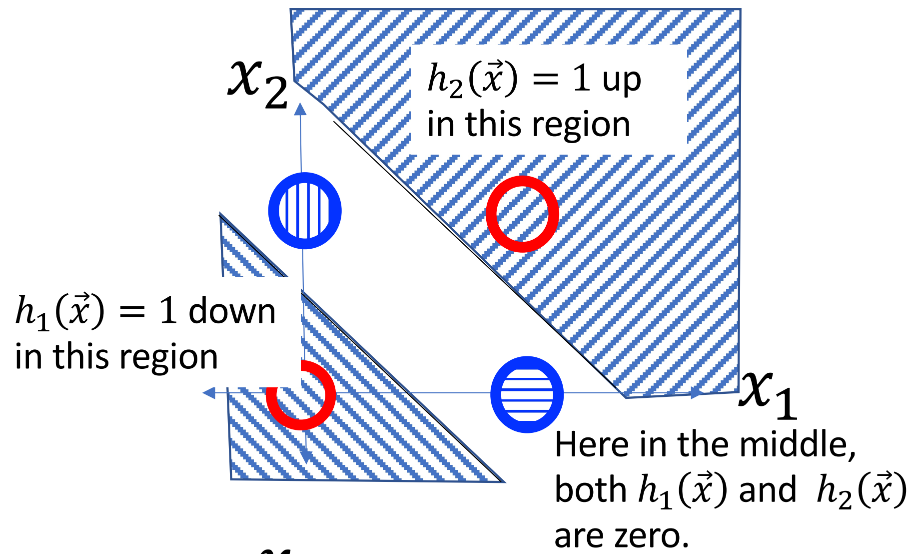
Suppose we create two **hidden nodes**:

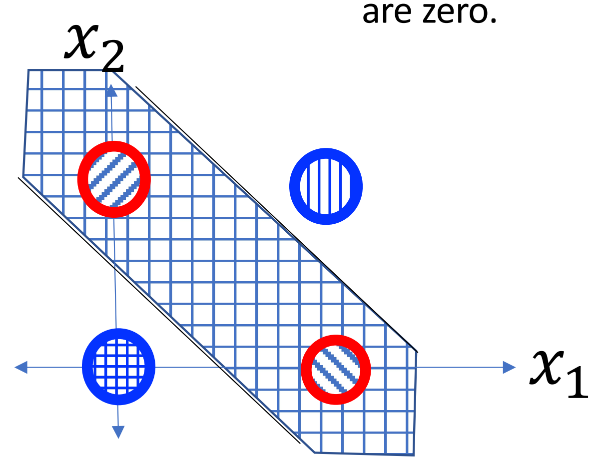
 $h_1(\vec{x}) = u(0.5 - x_1 - x_2)$

 $h_2(\vec{x}) = u(x_1 + x_2 - 1.5)$

Then **the XOR function** $f(\vec{x}) = (x_1 \oplus x_2)$ is given by $f(\vec{x}) = \neg(x_1 \vee x_2)$. For example, we could write this as:

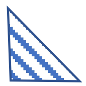
 $f(\vec{x}) = u\big(0.5 - h_1(x) - h_2(x)\big)$

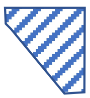


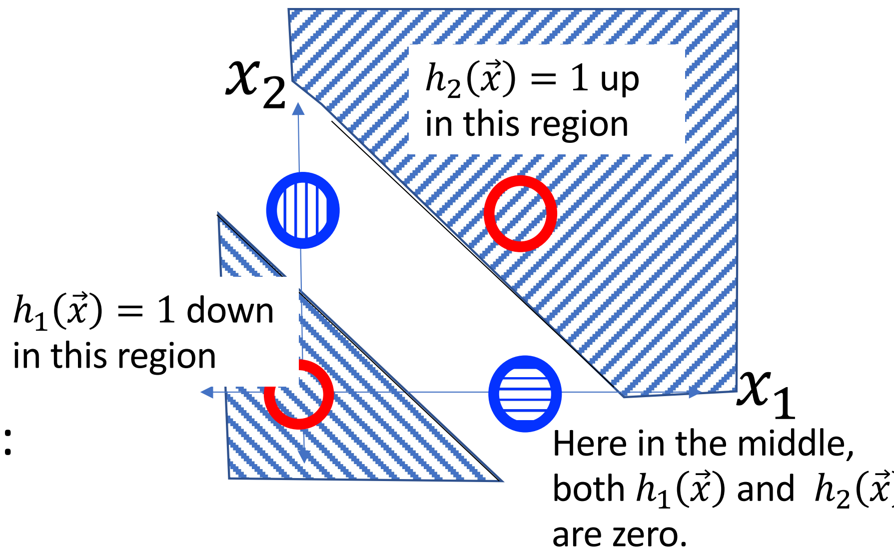


Flow diagrams

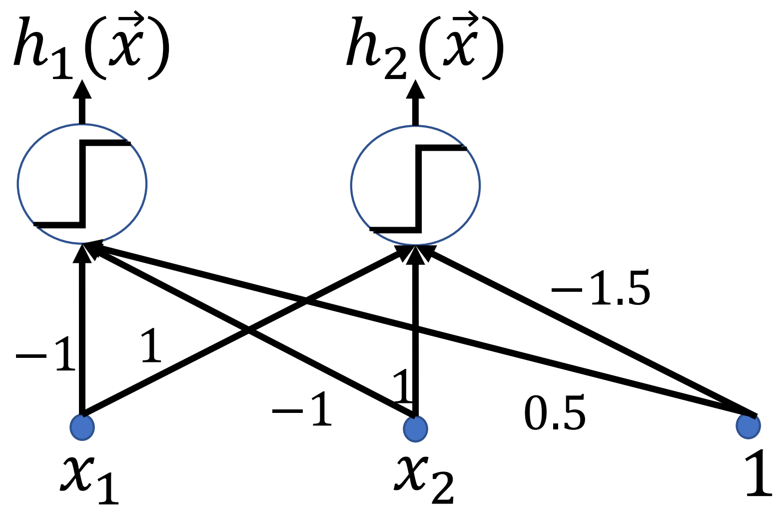
Suppose we create two **hidden nodes**:

 $h_1(\vec{x}) = u(0.5 - x_1 - x_2)$

 $h_2(\vec{x}) = u(x_1 + x_2 - 1.5)$



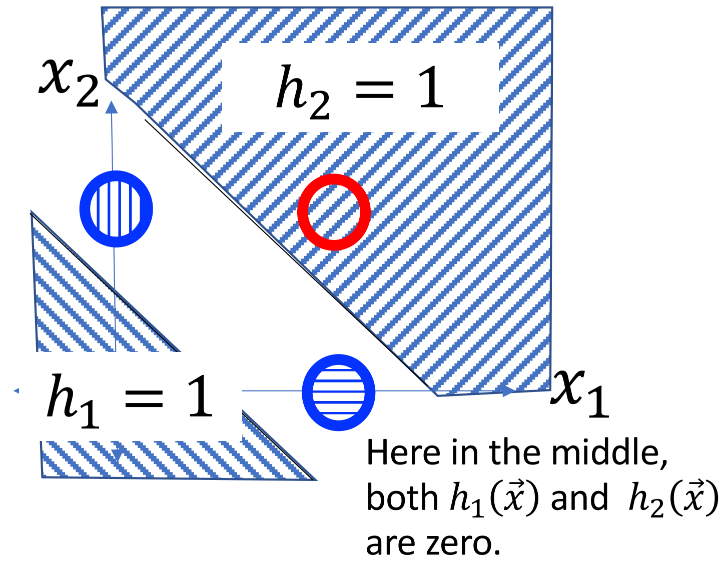
Here is a flow diagram for this computation:

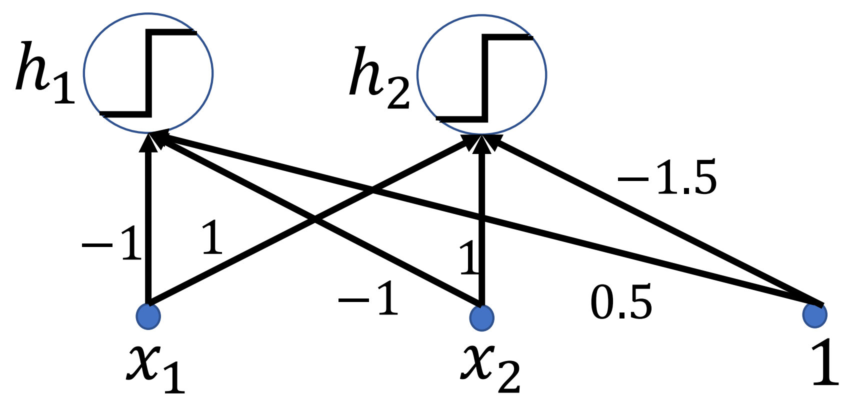


Flow diagrams

A flow diagram is a way to represent the computations performed by a neural network.

- Circles, a.k.a. "nodes," a.k.a. "neurons," represent scalar operations.
  - The circles above x_1 and x_2 represent the scalar operation of "read this datum in from the dataset."
  - The circles labeled h_1 and h_1 represent the scalar operation of "unit step function."
- Lines represent multiplication by a scalar.
- Where arrowheads come together, the corresponding variables are added.

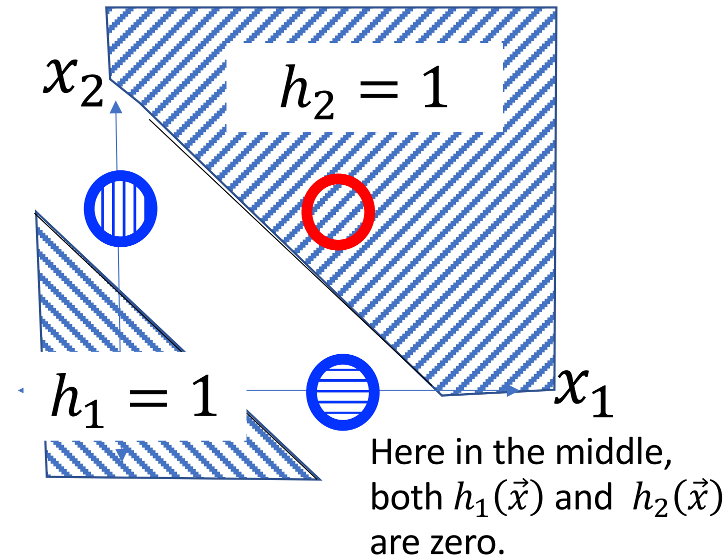


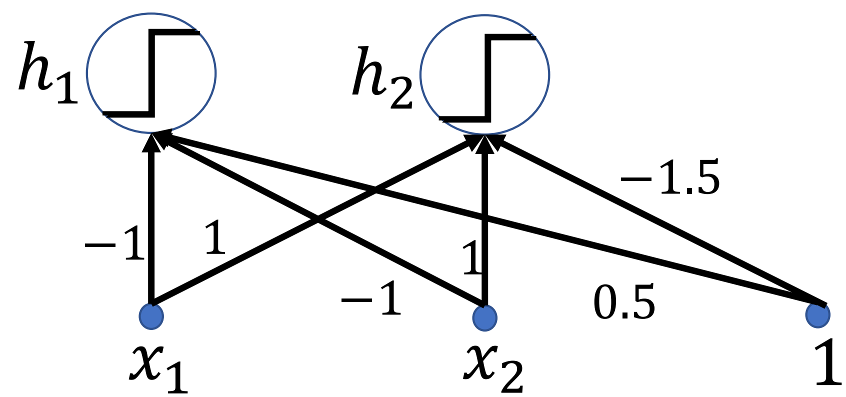


Flow diagrams

It's often useful to distinguish two types of hidden variables at each neuron:

- The neural excitation, ξ_j, is the result of adding together all of the inputs to the neuron.
- The neural activation, h_j, is the result of passing ξ_j through a scalar nonlinearity.

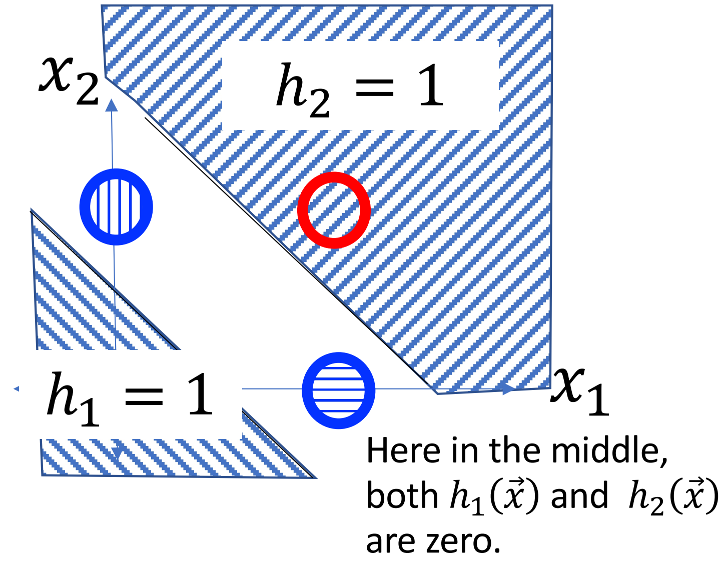




Flow diagrams

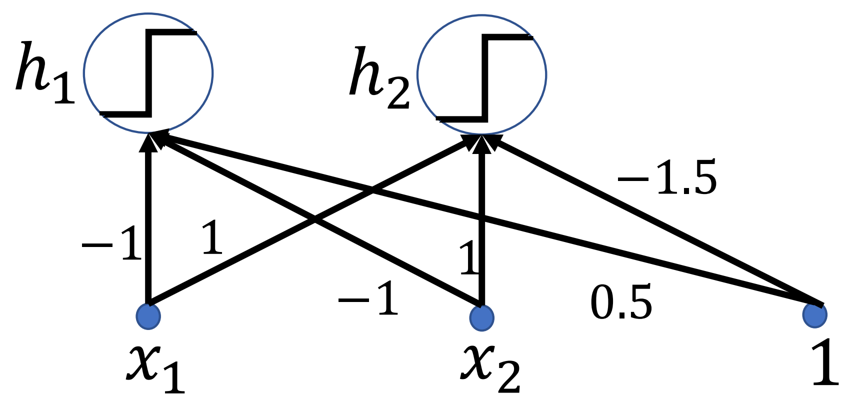
So in this flow diagram, for example, we can see that:

$$\xi_1 = 0.5 - 1 \cdot x_1 - 1 \cdot x_2$$
$$\xi_2 = -1.5 + 1 \cdot x_1 + 1 \cdot x_2$$



… and then …

$$h_1 = u(\xi_1)$$
$$h_2 = u(\xi_2)$$



… where $u(\cdot)$ is the unit step function.

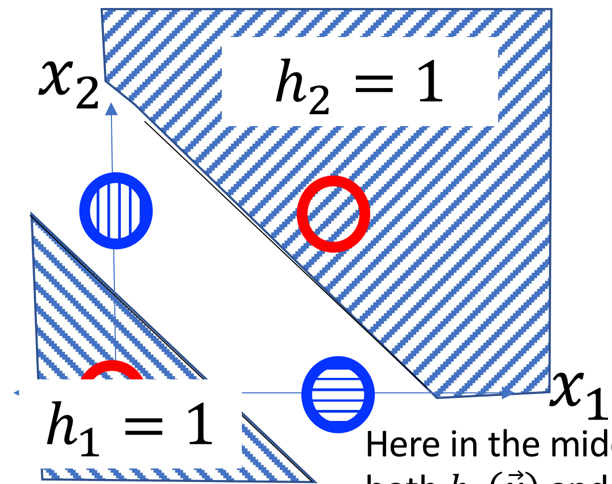
Flow diagrams

Now suppose that we want to compute

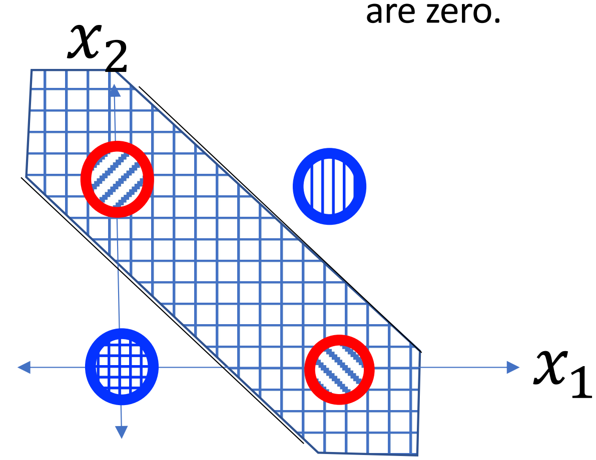
$f(\vec{x}) = (x_1 \oplus x_2)$. We could write this

as:

$$f(\vec{x}) = u(0.5 - h_1 - h_2)$$



Here in the middle, both $h_1(\vec{x})$ and $h_2(\vec{x})$ are zero.

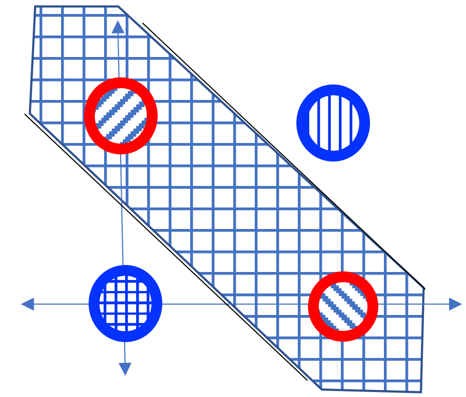


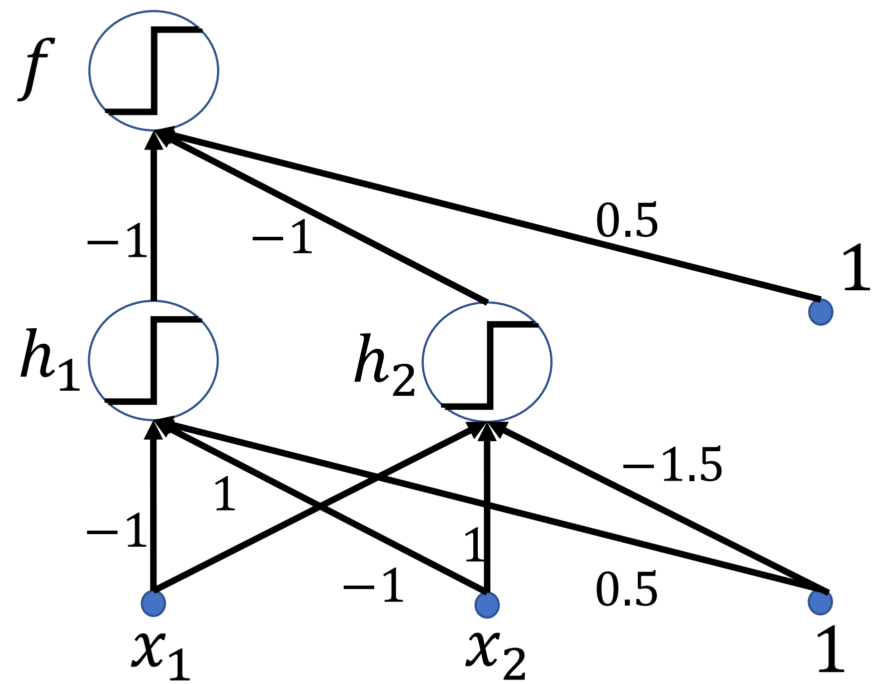
Flow diagrams

We can write the XOR function as:

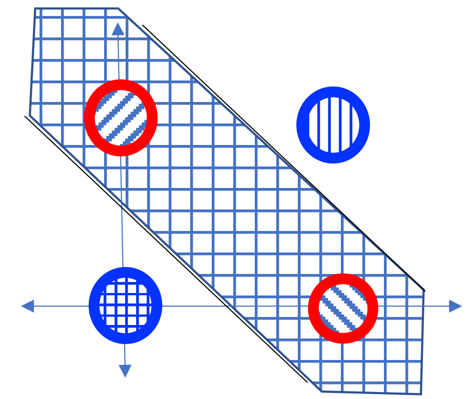
$$\xi_3 = 0.5 - 1 \cdot h_1 - 1 \cdot h_2$$

$$f(\vec{x}) = u(\xi_3)$$





Flow diagrams



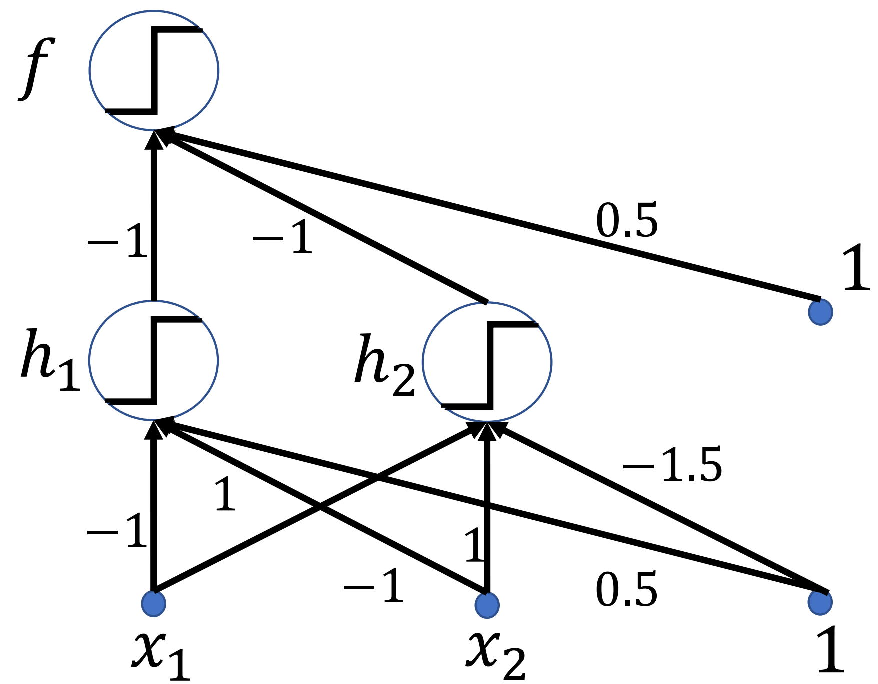
Putting it all together:

$$\xi_1 = 0.5 - 1 \cdot x_1 - 1 \cdot x_2$$
$$\xi_2 = -1.5 + 1 \cdot x_1 + 1 \cdot x_2$$

$$h_1 = u(\xi_1)$$
$$h_2 = u(\xi_2)$$

$$\xi_3 = 0.5 - 1 \cdot h_1 - 1 \cdot h_2$$

$$f(\vec{x}) = u(\xi_3)$$



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Multi-layer neural net

- $\xi_j^{(l)}$ = **excitation** of the j^th neuron (a.k.a. "node") in the l^th layer
  - Computed by adding together inputs from many other neurons, each weighted by a corresponding connection strength or connection weight, $w_{j,k}^{(l)}$
- $h_j^{(l)}$ = **activation** of the j^th node in the l^th layer
  - This is computed by just passing the excitation through a scalar nonlinear activation function, thus $h_j^{(l)} = g(\xi_j^{(l)})$. The activation functions in different layers differ, so to be pedantic, sometimes we'll write $h_j^{(l)} = g^{(l)}\left(\xi_j^{(l)}\right)$.

Multi-layer neural net

Given: some training token $\vec{x} = [x_1, \ldots, x_D, 1]^T$ and its target label y

1. Initialize: $h_k^{(0)} = x_k$
2. Forward propagate: for $l \in \{1, \ldots, L\}$:
   a. Compute the excitations as weighted sums of the previous-layer activations:
   $$\xi_j^{(l)} = b_j^{(l)} + \sum_k w_{j,k}^{(l)} h_k^{(l-1)}$$
   b. Compute the activations by applying scalar nonlinearities:
   $$h_j^{(l)} = g^{(l)}\left(\xi_j^{(l)}\right)$$
3. Output: $P(Y = k|x) \ = h_k^{(L)}$

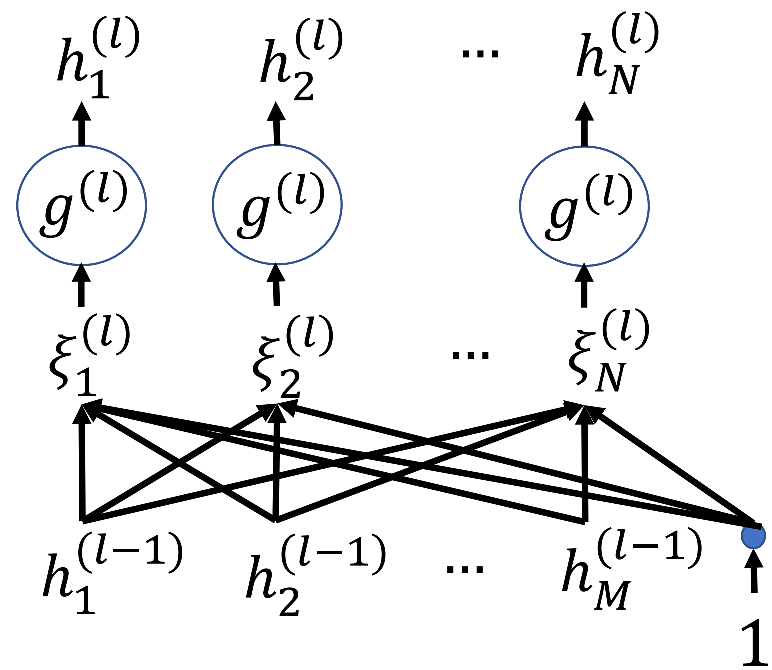
Forward propagation

- From activation to excitation is a matrix multiply:

$$\xi_j^{(l)} = b_j^{(l)} + \sum_k w_{j,k}^{(l)} h_k^{(l-1)}$$

- From excitation to activation is a scalar nonlinearity:

$$h_j^{(l)} = g^{(l)}\left(\xi_j^{(l)}\right)$$



Forward propagation: Matrix multiply

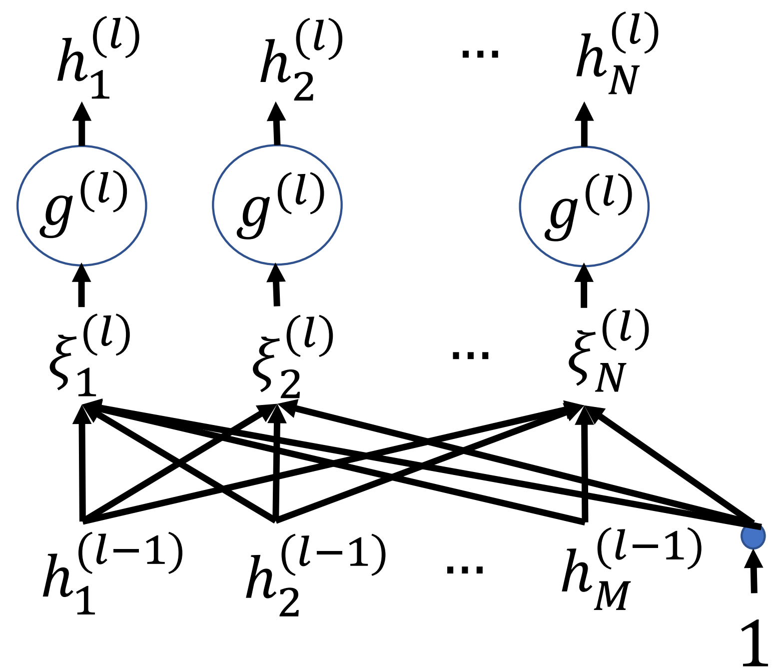
From activation to excitation is a matrix multiply:

$$\vec{\xi}^{(l)} = W^{(l)} \vec{h}^{(l-1)}$$

…where…

$$\vec{\xi}^{(l)} = \begin{bmatrix} \xi_1^{(l)} \\ \vdots \\ \xi_N^{(l)} \end{bmatrix}, \qquad \vec{h}^{(l-1)} = \begin{bmatrix} h_1^{(l-1)} \\ \vdots \\ h_M^{(l-1)} \\ 1 \end{bmatrix},$$

$$W^{(l)} = \begin{bmatrix} w_{1,1}^{(l)} & \cdots & w_{1,M}^{(l)} & b_1^{(l)} \\ \vdots & \ddots & \vdots & \vdots \\ w_{N,1}^{(l)} & \cdots & w_{N,M}^{(l)} & b_N^{(l)} \end{bmatrix}$$



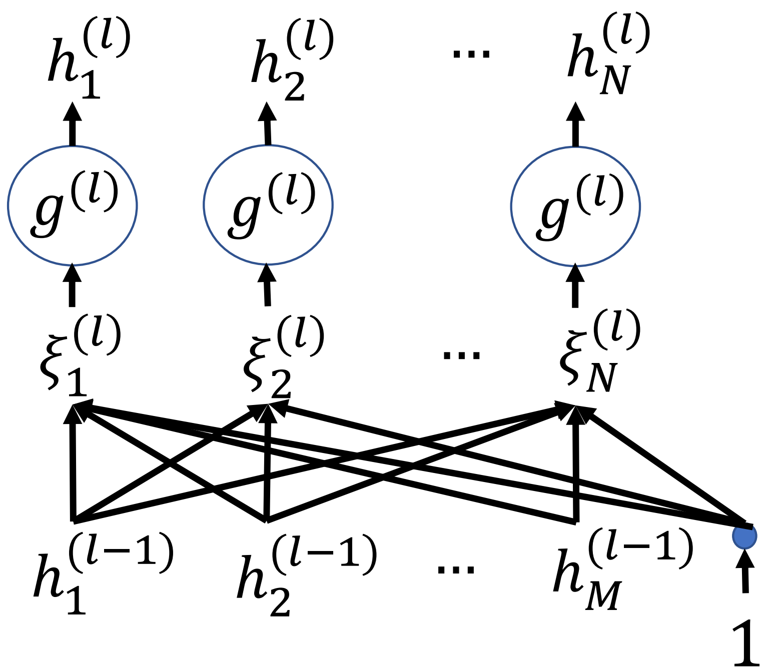
Forward propagation

From excitation to activation is a scalar nonlinearity:

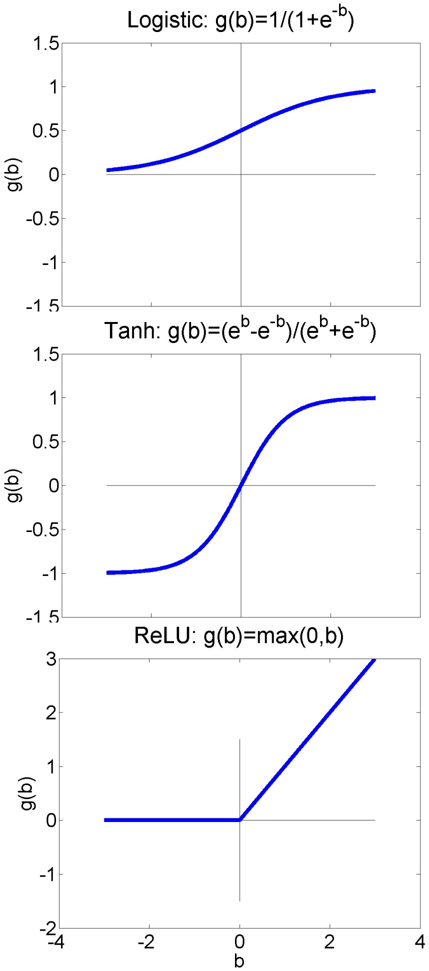
$$h_j^{(l)} = g^{(l)}\left(\xi_j^{(l)}\right)$$

What type of nonlinearity?

Answer: it depends on what task you want your neural net to learn.



Activation functions



The "activation function," $g^{(l)}(\cdot)$, can be any scalar nonlinearity. Common ones that you should know include the **unit step** and **signum** functions, and:

Logistic Sigmoid:

$$\sigma(\beta) = \frac{1}{1 + e^{-\beta}}$$

Hyperbolic Tangent (tanh):

$$\tanh(\beta) = \frac{e^{\beta} - e^{-\beta}}{e^{\beta} + e^{-\beta}}$$

Rectified Linear Unit (ReLU):

$$\text{ReLU}(\beta) = \max(0, \beta)$$

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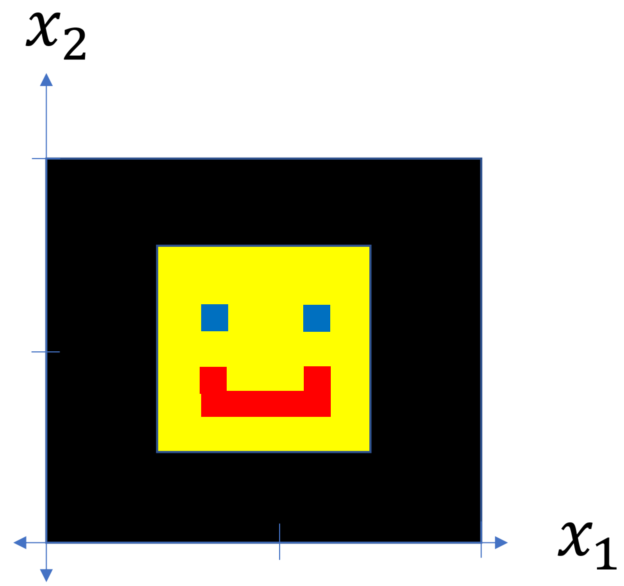
Example: Square smiley

- Input: $\vec{x} = [x_1, x_2, 1]^T$
- Output: $f(\vec{x}) = [R, G, B]^T$

Remember that yellow = red + green, so we just need to compute R, G, B as functions of x_1 and x_2.

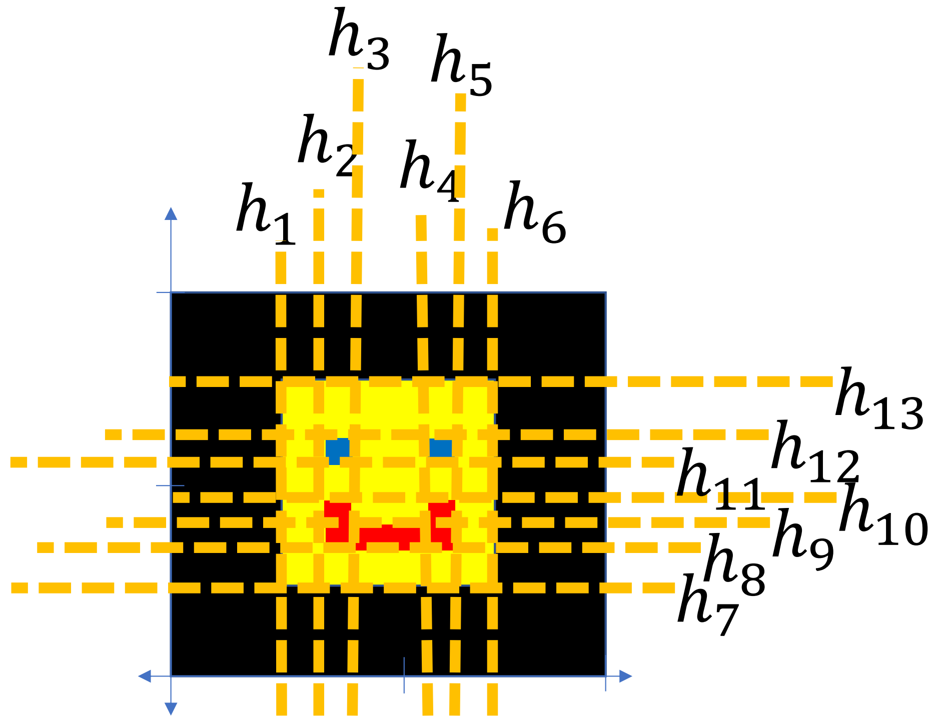
This could be done using a two-layer network, but I it's easier using a three-layer network, so let's do it that way.



Layer 1

In layer 1, let's find all the different ways in which we need to bisect the image plane:

$$h_1^{(1)} = \text{sign}(x_1 - 0.5)$$
$$\vdots$$
$$h_{13}^{(1)} = \text{sign}(x_2 - 1.5)$$



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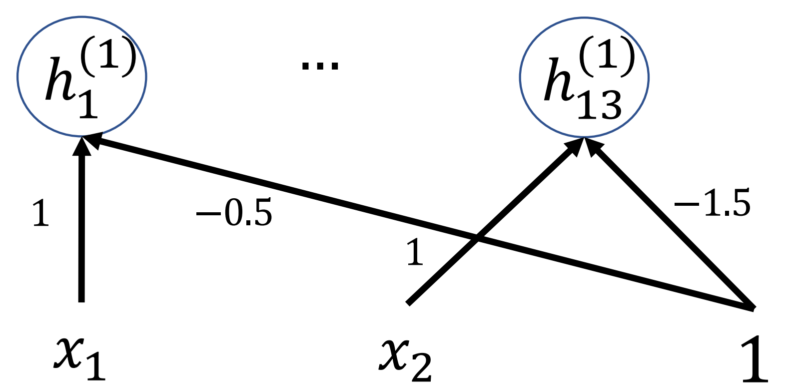
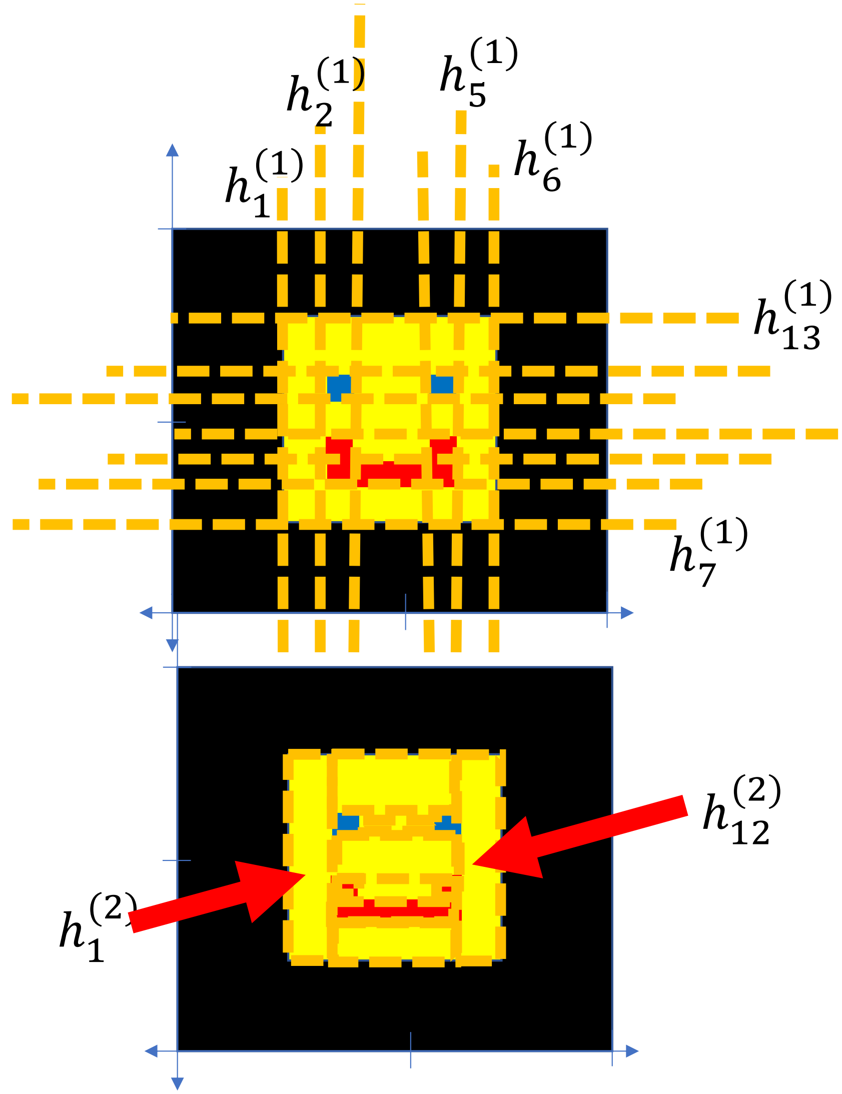


Layer 2

In layer 2, let's compute rectangles of solid color. We can compute those using logical operations:

$$h_1^{(2)} = h_1^{(1)} \land \neg h_2^{(1)} \land h_7^{(1)} \land \neg h_{13}^{(1)}$$
$$\vdots$$
$$h_{12}^{(2)} = h_5^{(1)} \land \neg h_6^{(1)} \land h_7^{(1)} \land \neg h_{13}^{(1)}$$



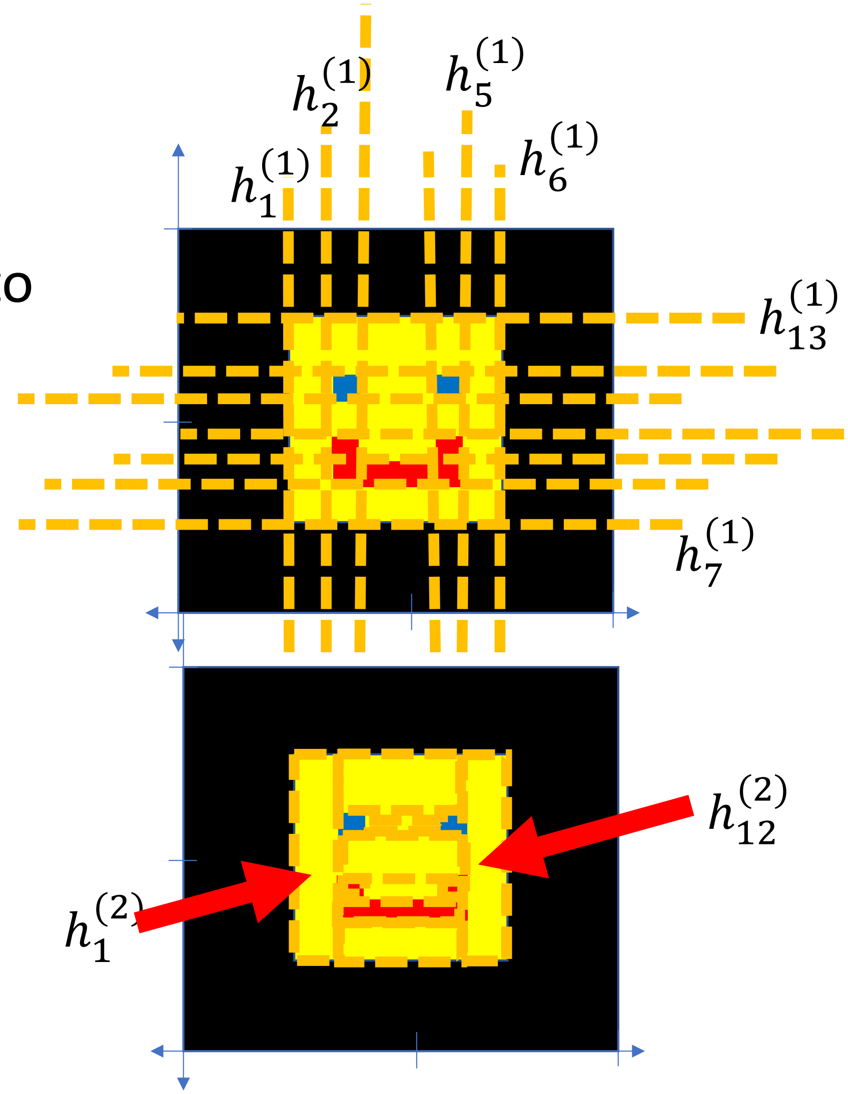
Layer 2

… and then convert the logical operations into linear functions:

$$h_1^{(2)} = \mathrm{u}\left(h_1^{(1)} - h_2^{(1)} + h_7^{(1)} - h_{13}^{(1)} - 3.5\right)$$

$$\vdots$$

$$h_{12}^{(2)} = \mathrm{u}\left(h_5^{(1)} - h_6^{(1)} + h_7^{(1)} - h_{13}^{(1)} - 3.5\right)$$



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$$h_1^{(2)} = \mathrm{u}\left(h_1^{(1)} - h_2^{(1)} + h_7^{(1)} - h_{13}^{(1)} - 3.5\right)$$
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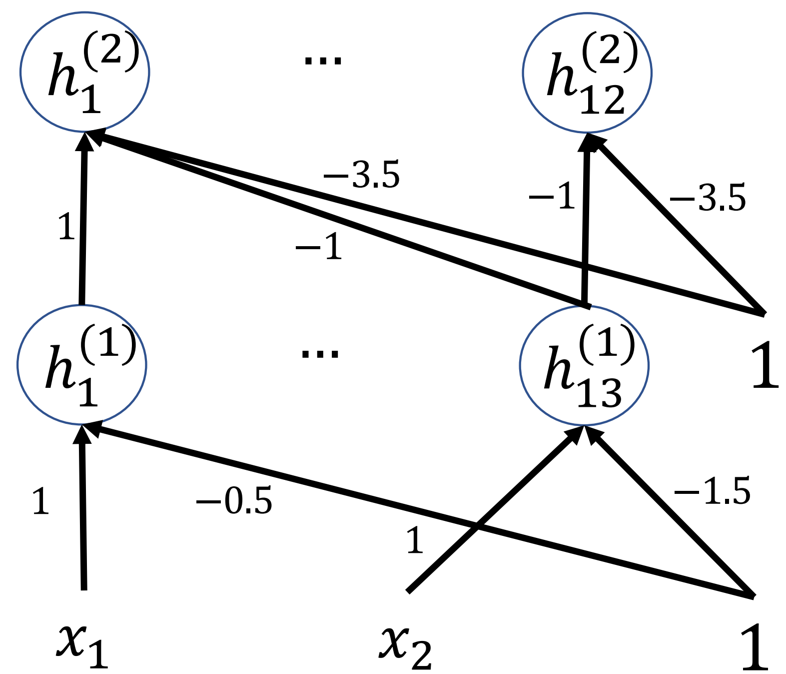
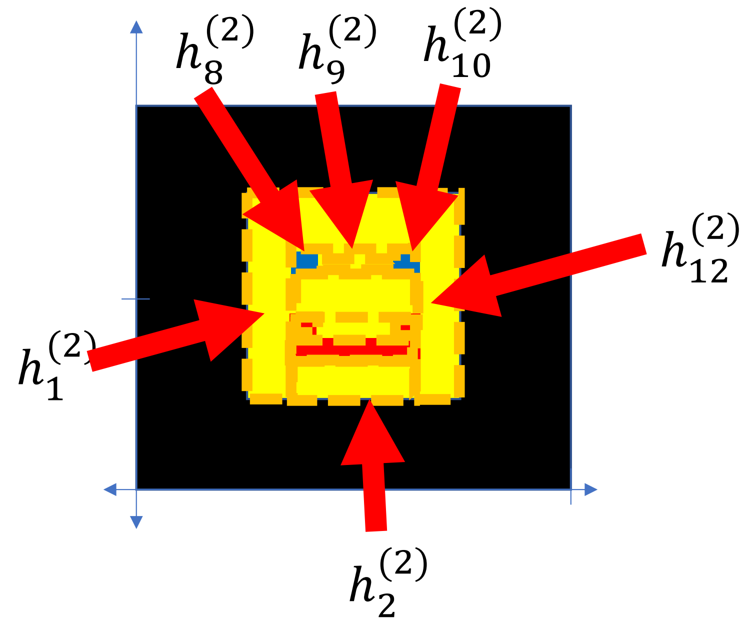


Layer 3

In layer 3, let's compute the red, green, and blue regions using the inclusive-OR of these rectangles:



$$R = h_1^{(2)} \vee h_2^{(2)} \vee h_3^{(2)} \vee h_4^{(2)} \vee h_5^{(2)} \vee h_6^{(2)} \vee h_7^{(2)} \vee h_9^{(2)} \vee h_{11}^{(2)} \vee h_{12}^{(2)}$$

$$G = h_1^{(2)} \vee h_2^{(2)} \vee h_5^{(2)} \vee h_7^{(2)} \vee h_9^{(2)} \vee h_{11}^{(2)} \vee h_{12}^{(2)}$$

$$B = h_8^{(2)} \vee h_{10}^{(2)}$$

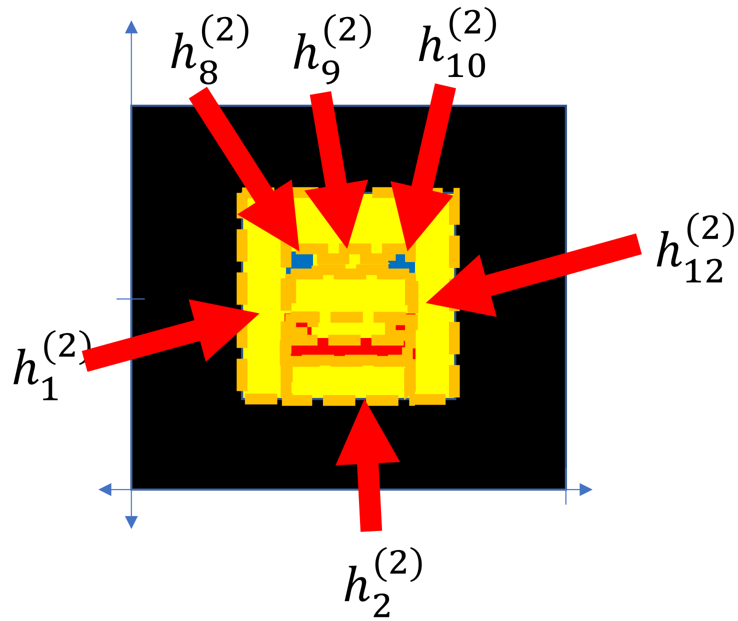
Layer 3

In layer 3, let's compute the red, green, and blue regions using the inclusive-OR of these rectangles:

$$R = u\begin{pmatrix} h_1^{(2)} + h_2^{(2)} + h_3^{(2)} + h_4^{(2)} + h_5^{(2)} \\ +h_6^{(2)} + h_7^{(2)} + h_9^{(2)} + h_{11}^{(2)} + h_{12}^{(2)} - 0.5 \end{pmatrix}$$

$$G = u\begin{pmatrix} h_1^{(2)} + h_2^{(2)} + h_5^{(2)} + h_7^{(2)} + h_9^{(2)} + \\ h_{11}^{(2)} + h_{12}^{(2)} - 0.5 \end{pmatrix}$$

$$B = \mathrm{u}\left(h_8^{(2)} + h_{10}^{(2)} - 0.5\right)$$



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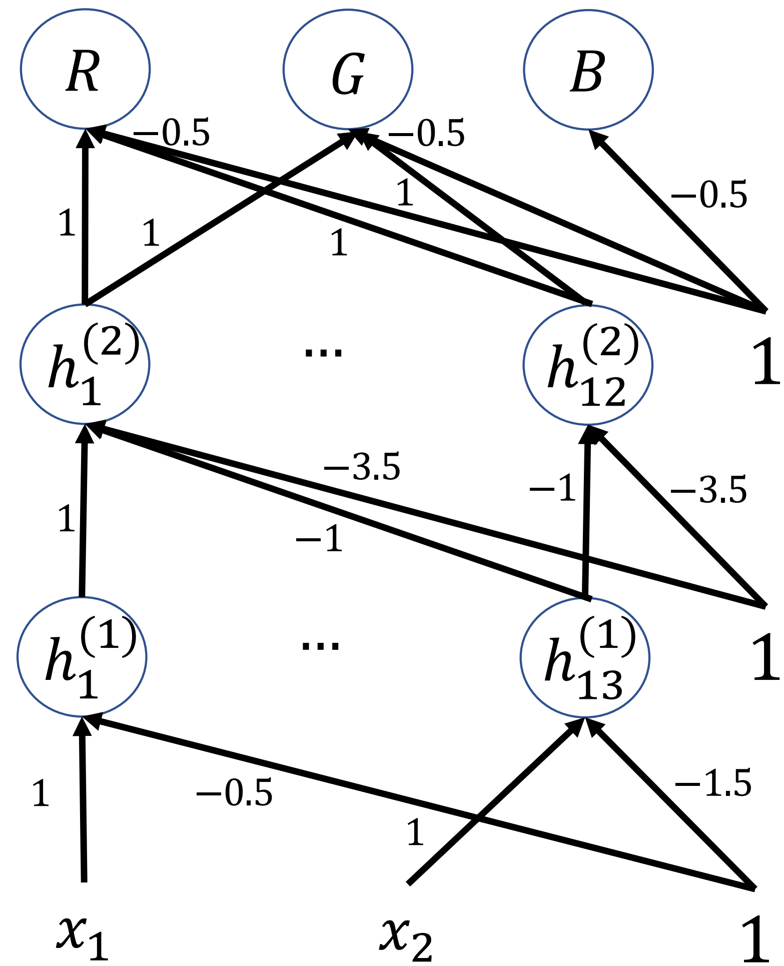
$$R = u\begin{pmatrix} h_1^{(2)} + h_2^{(2)} + h_3^{(2)} + h_4^{(2)} + h_5^{(2)} \\ +h_6^{(2)} + h_7^{(2)} + h_9^{(2)} + h_{11}^{(2)} + h_{12}^{(2)} - 0.5 \end{pmatrix}$$

$$G = u\begin{pmatrix} h_1^{(2)} + h_2^{(2)} + h_5^{(2)} + h_7^{(2)} + h_9^{(2)} + \\ h_{11}^{(2)} + h_{12}^{(2)} - 0.5 \end{pmatrix}$$

$$B = \mathrm{u}\left(h_8^{(2)} + h_{10}^{(2)} - 0.5\right)$$



Summary

- Breaking the constraints of linearity: multi-layer neural nets
- Flow diagram for the XOR problem: if x_1 and x_2 are binary, then

$$(x_1 \vee x_2) = u(x_1 + x_2 - 0.5)$$
$$(x_1 \wedge x_2) = u(x_1 + x_2 - 1.5)$$

- Flow diagram for a multi-layer neural net

$$\xi_j^{(l)} = b_j^{(l)} + \sum_k w_{j,k}^{(l)} h_k^{(l-1)}$$
$$h_j^{(l)} = g^{(l)}\left(\xi_j^{(l)}\right)$$

- Forward-propagation example